

Phase Transitions in Three-Dimensional Bosonic Optical Lattices

H. Kleinert^{a,*}, Z. Narzikulov^{b,†} and Abdulla Rakhimov^{a,b,‡}

^a *Institut für Theoretische Physik, Freie Universität Berlin,*

Arnimallee 14, D-14195 Berlin, Germany

^b *Institute of Nuclear Physics, Tashkent 100214, Uzbekistan*

Abstract

We develop the Collective Quantum Field Theory of $d = 3$ optical bosonic lattices and evaluate consequences at the mean-field level and in Variational Perturbation Theory (VPT). In contrast to a recent prediction for atomic gases by Cooper et. al. [14, 15], we find no superfluid state with zero condensate fraction.

*Electronic address: h.k@fu-berlin.de

†Electronic address: narzikulov@inp.uz

‡Electronic address: rakhimovabd@yandex.ru

I. INTRODUCTION

Optical lattices are gases of ultracold atoms trapped in periodic potentials created by periodically arranged intersecting standing waves of laser light. The interest in experimental and theoretical investigations of these artificial crystals is caused by the two following factors [1]:

1) Neutral atoms in these optical lattices have several of attractive features that make them interesting candidates for the realization of a quantum computer [2].

2) They may be used to simulate various lattice models of fundamental importance in condensed matter physics. Since they permit studying in a controlled way solid-state physics, in which one can fine-tune the interaction strength for various geometries of the lattices. In particular, it is possible to control the Hamiltonian parameters and study various regimes of system parameter.

The lattice of bosons with short - range repulsive pair interaction trapped in an optical lattice may be described by a Hamiltonian of Bose-Hubbard type:

$$H = -J \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{j}} + \frac{U}{2} \sum_{\mathbf{i}} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}} \hat{b}_{\mathbf{i}} + \sum_{\mathbf{i}} (\varepsilon_{\mathbf{i}} - \mu) \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}}, \quad (1)$$

where $\hat{b}_{\mathbf{i}}^{\dagger}$ and $\hat{b}_{\mathbf{i}}$ are the bosonic creation and annihilation operators on the site i ; the sum over $\langle \mathbf{i}, \mathbf{j} \rangle$ includes only pairs of nearest neighbors; J is the hopping amplitude, which is responsible for the tunneling of an atom from one site to another neighboring site; U is the on site repulsion energy, and N_s the number of sites.

At zero temperature with an integer *filling factor* $\nu \equiv N/N_s$, where N is the total number of atoms, a system of bosons described by the Hamiltonian (1) could be on superfluid (SF) or in Mott insulator (MI) phase. Clearly the quantum phase transition (QPT) between these two phases is allocated by the dimensionless interaction strength parameter $u = U/J$. For small u , the hopping term dominates the system, so that it prefers to be in the SF phase. For large $u \gg 1$, on the other hands, the system exhibits a MI phase.

A critical interaction strength $u_{\text{crit}} = 29.34$ was found for $d = 3$ by Monte Carlo calculations [3] at a filling factor $\nu = 1$, and agrees well with the experimental data [4].

To make for easier reading, we summarize some specific features of these two phases. The SF phase is characterized by a long-range correlation, a continuous (gapless) excitation spectrum and a finite compressibility. Since there exists a condensate with a finite number

of particles, n_0 , the gauge symmetry is spontaneously broken in accordance with theorems by Bogoliubov and Ginibre. In contrast, in the MI phase, there is no long-range correlation or breaking of gauge symmetry. The excitation spectrum has a gap and the system is incompressible, since there is a fixed number of atoms per-site. The mobility of atoms is completely different in the two phases. In the SF phase they can easily move from one site to another site by tunneling, whereas in the MI phase, they are localized.

Finite-temperature phases of optical lattices have been studied by Monte Carlo calculations as well as experimentally for $d = 3$. As expected, the system behaves as a normal fluid (NF) at $T > T_c$. A most interesting observation was made in Refs. [3, 4]: In contrast to the system of dilute Bose gases, the critical temperature is downshifted at the transition to the MI phase.

Most of present theoretical approaches can be divided into two classes which deal with the phase transitions SF \rightarrow MI and MI \rightarrow SF. The latter are based on the Ginzburg - Landau theory as described for instance in Ref. [5]. They are well suited for analyses of time-of-flight pictures of the condensates and the associated visibility at zero and finite temperatures. Although such approximation works well in MI phase, predicting Mott lobes with quantum phase boundaries, they can hardly be extended to the SF regime in practice. In the former class (SF \rightarrow MI) one uses a perturbative scheme [6] within a decoupling (or single site) approximation due to Gutzwiller, or within a mean field approximation. Gutzwiller variational approach which was first proposed for a fermion system [7], and further developed for bosons in Refs. [8, 9], has the following drawbacks [10]:

- The mean field Hamiltonian which features single boson terms does not conserve the total number of bosons [11];
- Tunneling of uncondensed atoms is neglected;
- The critical value u_{crit} does not depend on the lattice dimension.

The first application of a mean field approach was made in the Hartree - Fock-Popov (HFP) approximation to optical lattices by Stoof et. al. [12]. By studying the dependence of the condensate number n_0 on u , i.e. $n_0(U/J)$ they observed that n_0 never reaches zero even in the unitary limit ($u \rightarrow \infty$) implying that this approximation is unable to predict a QPT of SF \rightarrow MI. In contrast to this, the two-loop approximation by present authors in [13]

suggests the existence of such a QPT , but the critical value of u_{crit} was found to be rather small: $u_{\text{crit}}(\text{two-loop}) \approx 6$ for $d = 3$. So, the question about the ability of approximations, based on mean field theory to describe phase diagrams of optical lattices adequately remains still open.

A new approximation has been recently made by Fred Cooper et al. [14, 15] in the treatment of dilute Bose gases. They found a simple way of fixing the degeneracy in the elimination of the interaction by auxiliary collective pair and density fields via standard Hubbard - Stratonovitch transformations. Although their approach gives no QPT for a homogenous Bose gas at zero temperature, it predicts a desirable second order BEC transition at finite temperatures and exhibits a positive shift in the critical temperature T_c that is consistent with Monte Carlo and other calculations [16, 17]. One of the novel features of that calculations is that for $T < T_c$ it predicts a novel type of superfluid phase that does not have a condensate [18]. Although such a phase has not been observed yet, it was justified by the existence of a nonzero anomalous density δ , in the region $T_c < T \leq T^*$, where T^* is the transition temperature to the normal phase .

In the present work we shall formulate a similar two-collective quantum field theory for discrete systems such as optical lattices and ask the following questions

- Does it predict a SF \rightarrow MI quantum phase transition?
- Does it predict the suppression of T_c at large u ?
- Does it predict a new phase , mentioned above, for optical lattices either?

Our results will be compared with those of another well-known mean-field approximation, the Hartree - Fock - Bogoliubov (HFB) approximation, which is widely used to describe BEC in homogeneous Bose gases and in triplons [19, 20] in magnetic insulators, and will also be extended here to optical lattices.

The paper is organized as follows. In Sections II and III we shall derive Collective Quantum Field Theory and HFB approaches for optical lattices, respectively. The results and discussions will be presented in Section IV, and the conclusions will be stated in Section V.

II. COLLECTIVE QUANTUM FIELD THEORY OF 3D BOSE-HUBBARD MODEL

In the Wannier representation the Euclidian action, corresponding to the Bose - Hubbard Hamiltonian is given by [13]

$$\begin{aligned} \mathcal{A}(\psi^*, \psi) = & \int_0^\beta d\tau \left\{ \sum_{\mathbf{i}} \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) [\partial_\tau - \mu] \psi(\mathbf{x}_{\mathbf{i}}, \tau) - J \sum_{\langle i, j \rangle} \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{j}}, \tau) \right. \\ & \left. + \frac{U}{2} \sum_{\mathbf{i}} \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{i}}, \tau) \right\}, \end{aligned} \quad (2)$$

where μ is the chemical potential and $\beta = 1/T$. The lattice points lie at the positions [21]

$$\mathbf{x}_{\mathbf{i}} = \mathbf{i} a, \quad (3)$$

where a is the lattice spacing, and

$$\mathbf{i} \equiv (i_1, i_2, \dots, i_d), \quad (4)$$

are integer-valued vectors.

The partition function Z , and the grand thermodynamic potential Ω , can be found as:

$$Z = \int D\psi^* D\psi e^{-\mathcal{A}(\psi^*, \psi)}, \quad (5)$$

$$\Omega = -T \ln Z. \quad (6)$$

The ground state expectation value of an operator $\hat{O}(\psi^*, \psi)$ can be expressed as a functional integral:

$$\langle \hat{O} \rangle = \frac{1}{Z} \int \mathcal{D}\psi^* \mathcal{D}\psi \hat{O}(\psi^*, \psi) e^{-\mathcal{A}(\psi^*, \psi)}. \quad (7)$$

With the help of a Hubbard - Stratonovich transformation, the interaction term in (2) can be eliminated by adding to the action in the exponent of (5) a dummy functional integral $\int \mathcal{D}\Delta \mathcal{D}\Delta^* e^{-\mathcal{A}_{\text{pair}}}$ containing a pair field Δ with following action [22]:

$$\mathcal{A}_{\text{pair}} = \int_0^\beta d\tau \sum_{\mathbf{i}} \left\{ \frac{1}{2U} \left| \Delta(\mathbf{x}_{\mathbf{i}}, \tau) - U \psi(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{i}}, \tau) \right|^2 \right\}. \quad (8)$$

A functional integral over Δ, Δ^* produces an irrelevant multiplication of the partition function Z by a trivial constant factor.

It has been emphasized in [22] and the textbook [23] that this procedure is highly degenerate. Instead of (8) one could just as well have introduced a plasmon field by adding to

the action in the exponent of (5) the dummy functional integral containing a density field φ with following action

$$\mathcal{A}_{\text{pl}} = \int_0^\beta d\tau \sum_{\mathbf{i}} \left\{ -\frac{1}{2U} (\varphi(\mathbf{x}_{\mathbf{i}}, \tau) - U\psi^*(\mathbf{x}_{\mathbf{i}}, \tau)\psi(\mathbf{x}_{\mathbf{i}}, \tau))^2 \right\}. \quad (9)$$

Diagrammatically, the degeneracy is caused by the fact that the sum of all collective field diagrams will always produce the same result if evaluated to *all* orders in perturbation theory. Each of these collective fields reproduces all effects of the interaction if it is integrated functionally. A difference appears, if the evaluation is restricted to a mean-field approximation. Then it depends on the dominance of certain dynamical effects which field is preferable.

In principle, we can also add a combination of $\mathcal{A}_{\text{pair}}$ and \mathcal{A}_{pl} , and still leave the physical properties of the system unchanged. For instance $\cosh^2 \theta \mathcal{A}_{\text{pl}} - \sin^2 \theta \mathcal{A}_{\text{pair}}$. Diagrammatically, however, the degeneracy cannot be easily verified since a calculation of the diagrams to all order is really impossible. It can only be done to some finite order, for instance in a loop expansion, so that the mathematical equivalence is initially of little use.

One method to avoid the degeneracy and make the collective field approach unique has been pointed out a long time ago. It is based on an extension of the standard effective potential approach from $\mathcal{A}[\Psi^*, \Psi]$, whose expansion terms are the one-particle irreducible vertex functions of the theory. A unique version of collective fields can be introduced by going to a *higher effective action* $\mathcal{A}[\Psi^*, \Psi, \Delta, \Delta^*, \varphi]$. While the ordinary effective action $\mathcal{A}[\Psi^*, \Psi]$ is derived from a Legendre transformation of the generating functional of the theory $W[\eta, \eta^*]$ in which additional source terms $\eta\psi^* + \eta^*\psi$ have been added to the action, the higher effective action is obtained from the Legendre transformation of a generating functional $W[\eta, \eta^*, j, K, K^*]$ in which additional sources have been added to the action coupled to the density and the pair fields. The higher effective action will depend on the expectations of the fields $\psi, \psi^*, \rho \propto \psi^*\psi, \Delta \propto \psi\psi$ and $\Delta^* \propto \psi^*\psi^*$. At the end, it must merely be *extremized*, and no extra functional integrals [24] can cause any double-counting of Feynman diagrams. The expansion terms in the higher effective action are the two-particle irreducible vertex functions of the theory.

Another method that also abandons the fluctuations of the collective fields in favor of a collective classical field has been developed in recent years from a generalization of a variational approach to path integrals [25] to all orders in perturbation theory. It was

extremely successful and has led to the most accurate theory of critical phenomena [26] so far, named Variational Perturbation Theory (VPT) (for a review paper see [27]).

A third method which has recently been proposed and applied [14, 15] uses the combination of both fully fluctuating collective fields implied by the above dummy action $\cosh^2 \theta \mathcal{A}_{\text{pl}} - \sin^2 \theta \mathcal{A}_{\text{pair}}$ for the particular value $\sinh \theta = 1$. This choice is preferable if we want the mean-field approximation to exhibit excitations that have no energy gap, to comply with the Nambu-Goldstone theorem. After a trivial change of the normalization of plasmon and pair fields in the total action $\mathcal{A} + \cosh^2 \mathcal{A}_{\text{pl}} - \mathcal{A}_{\text{pair}}$ one arrives at

$$\mathcal{A} = \mathcal{A}_\psi[\psi^*, \psi] + \mathcal{A}_\varphi[\varphi] + \mathcal{A}_\Delta[\Delta, \Delta^*], \quad (10)$$

with

$$\begin{aligned} \mathcal{A}_\psi[\psi^*, \psi] = & \int_0^\beta d\tau \sum_{\mathbf{i}} \{ \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) [\partial_\tau - \mu + \cosh \theta \varphi(\mathbf{x}_{\mathbf{i}}, \tau)] \psi(\mathbf{x}_{\mathbf{i}}, \tau) \\ & - \frac{1}{2} \sinh \theta [\Delta \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{i}}, \tau) + \Delta^* \psi(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{i}}, \tau)] \} - J \int_0^\beta d\tau \sum_{\mathbf{i}, \mathbf{j}} \psi^*(\mathbf{x}_{\mathbf{i}}, \tau) \psi(\mathbf{x}_{\mathbf{j}}, \tau), \end{aligned} \quad (11)$$

$$\mathcal{A}_\varphi[\varphi] = - \int_0^\beta d\tau \sum_{\mathbf{i}} \frac{\varphi^2(\mathbf{x}_{\mathbf{i}}, \tau)}{2U}, \quad \mathcal{A}_\Delta[\Delta, \Delta^*] = \int_0^\beta d\tau \sum_{\mathbf{i}} \frac{\Delta(\mathbf{x}_{\mathbf{i}}, \tau) \Delta^*(\mathbf{x}_{\mathbf{i}}, \tau)}{2U}. \quad (12)$$

At the level of for fully fluctuating fields φ , Δ , Δ^* , the parameter θ is still arbitrary. The enforcement of the Nambu-Goldstone theorem will fix the parameter θ to make $\sin \theta = 1$.

Now we consider separately two regions, with and without a condensed phase.

A. Condensed phase

In this phase, the $U(1)$ gauge symmetry is spontaneously broken. It can be studied after a Bogoliubov shift of the field [10]

$$\psi(x_{\mathbf{i}}, \tau) = \psi_0 + \tilde{\psi}(x_{\mathbf{i}}, \tau), \quad (13)$$

with

$$\psi_0 = \sqrt{\nu n_0}. \quad (14)$$

where the $n_0 = N_0/N$ is the condensate fraction. It is a constant in the absence of a magnetic trap. The fluctuating field $\tilde{\psi}(x, \tau)$ must satisfy the condition:

$$\int_0^\beta d\tau \sum_{\mathbf{i}} \tilde{\psi}(x_{\mathbf{i}}, \tau) = 0. \quad (15)$$

Substituting (13) into (11), and decomposing the quantum field $\tilde{\psi}(\mathbf{x}_i, t)$ into its real and imaginary parts $\psi_1(\mathbf{x}_i, t)$ and $\psi_2(\mathbf{x}_i, t)$ as

$$\tilde{\psi}(\mathbf{x}_i, t) = \frac{1}{\sqrt{2}}(\psi_1(\mathbf{x}_i, t) + i\psi_2(\mathbf{x}_i, t)), \quad \tilde{\psi}^*(\mathbf{x}_i, t) = \frac{1}{\sqrt{2}}(\psi_1(\mathbf{x}_i, t) - i\psi_2(\mathbf{x}_i, t)), \quad (16)$$

we may separate the action as follows:

$$\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_2 + \mathcal{A}_\Delta + \mathcal{A}_\varphi, \quad (17)$$

with

$$\mathcal{A}_0 = -N_s \beta \nu n_0 (\mu + J z_0) + \nu n_0 \sum_{\mathbf{i}} \int_0^\beta d\tau [\cosh \theta \varphi(x_{\mathbf{i}}, \tau) - \frac{1}{2} \sinh \theta (\Delta(x_{\mathbf{i}}, \tau) + \Delta^*(x_{\mathbf{i}}, \tau))], \quad (18)$$

$$\mathcal{A}_2 = \frac{1}{2} \sum_{\mathbf{i}} \int_0^\beta d\tau \sum_{a,b=1,2} [i\varepsilon_{ab} \tilde{\psi}_a(x_{\mathbf{i}}, \tau) \partial_\tau \tilde{\psi}_b(x_{\mathbf{i}}, \tau) + \tilde{\psi}_a(x_{\mathbf{i}}, \tau) X_a \tilde{\psi}_b(x_{\mathbf{i}}, \tau) \delta_{ab}] \quad (19)$$

$$- \frac{J}{2} \int_0^\beta d\tau \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \sum_a \tilde{\psi}_a(x_{\mathbf{i}}, \tau) \tilde{\psi}_a(x_{\mathbf{j}}, \tau), \quad (20)$$

where \mathcal{A}_Δ and \mathcal{A}_φ are given in (12), ε_{ab} is an antisymmetric tensor with $\varepsilon_{12} = -\varepsilon_{21} = 1$, $z_0 = 2d = 6$, and

$$\begin{aligned} X_1 &= -\mu + \varphi(x_{\mathbf{i}}, \tau) \cosh \theta - \frac{1}{2} \sinh \theta (\Delta^*(x_{\mathbf{i}}, \tau) + \Delta(x_{\mathbf{i}}, \tau)), \\ X_2 &= -\mu + \varphi(x_{\mathbf{i}}, \tau) \cosh \theta + \frac{1}{2} \sinh \theta (\Delta^*(x_{\mathbf{i}}, \tau) + \Delta(x_{\mathbf{i}}, \tau)). \end{aligned} \quad (21)$$

For a homogenous, system the condensate is uniform and it is convenient to decompose the fluctuations into a Fourier series as [28, 29]

$$\tilde{\psi}_a(\mathbf{x}_i, \tau) = \frac{1}{\beta \sqrt{N_s^d}} \sum'_{\mathbf{q}, \omega_n} \int_0^\beta \psi_a(\mathbf{q}, \omega_n) e^{-i\omega_n \tau} \exp[i\mathbf{x}_i \mathbf{p}_\mathbf{q}] \quad (22)$$

where $\omega_n = 2\pi nT$ are Matsubara frequencies, and $\mathbf{p}_\mathbf{q} \equiv \{q_1, q_2, \dots, q_d\} 2\pi/N_s a$, with q_i running from 1 to $N_s - 1$ are the discrete-valued momentum vectors in the Brillouin zone. The momentum sum is explicitly

$$\frac{1}{N_s} \sum'_{\mathbf{q}} \equiv \frac{1}{N_s^d} \sum_{q_1=0}^{N_s-1} \sum_{q_2=0}^{N_s-1} \cdots \sum_{q_d=0}^{N_s-1}. \quad (23)$$

The prime on the symbol indicates that the $\mathbf{p} = 0$ -mode is omitted since it is contained in the subtracted ψ_0 . This will be useful to avoid possible infrared divergencies, especially for $d < 3$.

In momentum space, the quadratic term \mathcal{A}_2 reads

$$\mathcal{A}_2 = \frac{1}{2} \sum_{\mathbf{q}, \mathbf{q}', m, n} \psi_a(\mathbf{q}, \omega_n) G_{ab}^{-1}(\mathbf{q}, \omega_n; \mathbf{q}', \omega_m) \psi_b(\mathbf{q}', \omega_m), \quad (24)$$

with the propagator

$$G(\omega_n, \mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} \begin{pmatrix} \varepsilon(\mathbf{q}) + X_2 - Jz_0 & \omega_n \\ -\omega_n & \varepsilon(\mathbf{q}) + X_1 - Jz_0 \end{pmatrix}, \quad (25)$$

where the bare dispersion $\varepsilon(\mathbf{q})$ and phonon dispersion $\mathcal{E}(\mathbf{q})$ are given by

$$\varepsilon(\mathbf{q}) = 2J \left(d - \sum_{\alpha=1}^d \cos(2\pi q_\alpha / N_s) \right), \quad (26)$$

$$\mathcal{E}(\mathbf{q}) = \sqrt{(X_1 + \varepsilon(\mathbf{q}) - Jz_0)(X_2 + \varepsilon(\mathbf{q}) - Jz_0)}. \quad (27)$$

In the long-wavelength limit, $\varepsilon(\mathbf{q})$ behaves like

$$\varepsilon(\mathbf{q}) = J \frac{4\pi^2}{N_s^2} \mathbf{q}^2 = Ja^2 \mathbf{p}^2 + \dots \quad (28)$$

By comparison with the usual momentum-dependence of a free single-particle energy $\mathbf{p}^2/2M$ we identify the particle mass $M = 1/2Ja^2$.

Note that in coordinate space the Green function is defined by

$$\begin{aligned} G_{ab}(\mathbf{x}_i, \tau; \mathbf{x}_j, \tau') &\equiv G_{ab}(\mathbf{x}_i - \mathbf{x}_j, \tau - \tau') = \langle \psi_a(\mathbf{x}_i, \tau) \psi_b(\mathbf{x}_j, \tau') \rangle \\ &= \frac{1}{N_s \beta} \sum_n \sum_q e^{i\omega_n(\tau - \tau')} e^{i\mathbf{q}(\mathbf{x}_i - \mathbf{x}_j)} G_{ab}(\omega_n, \mathbf{q}). \end{aligned} \quad (29)$$

The thermodynamics of the system can be calculated from the partition function Z functional integral over all fields $\psi_1, \psi_2, \varphi, \Delta$ and Δ^* fields

$$Z = \int \mathcal{D}\psi_1 \mathcal{D}\psi_2 \mathcal{D}\varphi \mathcal{D}\Delta \mathcal{D}\Delta^* e^{-\mathcal{A}_0 - \mathcal{A}_2 - \mathcal{A}_\Delta - \mathcal{A}_\varphi}. \quad (30)$$

The first integrations by ψ_1 and ψ_2 are Gaussian and may be evaluated easily by using well-known formula

$$\begin{aligned} \int \mathcal{D}\psi_1 \mathcal{D}\psi_2 \exp \left[-\frac{1}{2} \sum_{a,b=1,2} \int \psi_a(x) G_{ab}^{-1}(x, y) \psi_b(y) dx dy - \int j_1(x) \psi_1(x) dx - \int j_2(x) \psi_2(x) dx \right] \\ = \sqrt{\text{Det } G} \exp \left[\sum_{a,b=1,2} \int j_a(x) G_{ab}(x, y) j_b(y) dx dy \right]. \end{aligned} \quad (31)$$

The integrations over the fluctuating collective fields, however, cannot be performed exactly, since they are nontrivially contained in $\sqrt{\text{Det } G}$. As usual in these circumstances, we resort to the saddle-point approximation [22, 30]. In the absence of a trap, we may assume the saddle point to lie at constant values of $\varphi(x_i, \tau)$ and $\Delta(x_i, \tau)$:

$$\begin{aligned} \varphi(x_i, \tau) &= \varphi_0, \\ \Delta(x_i, \tau) &= \Delta^*(x_i, \tau) = \Delta_0. \end{aligned} \quad (32)$$

Then the integrals over ψ_a become trivial and we may use the formula $\text{Det } G = e^{\text{Tr } \ln G}$ in Eqs. (30) and (31) to derive the following effective potential:

$$\Omega = \frac{T}{2} \sum_q \sum_n \ln(\omega_n^2 + \mathcal{E}^2(\mathbf{q})) + N_s \nu n_0 (\varphi' - \Delta) + \frac{N_s \Delta^2}{2U \sinh^2 \theta} - \frac{N_s (\varphi' + \mu + Jz_0)^2}{2U \cosh^2 \theta}, \quad (33)$$

with

$$\Delta \equiv \Delta \sinh \theta, \quad \varphi' = -\mu + \cosh \theta \varphi_0 - Jz_0. \quad (34)$$

The spectrum of density fluctuations is now from (27):

$$\mathcal{E}^2(\mathbf{q}) = (\varepsilon(\mathbf{q}) + \varphi' - \Delta)(\varepsilon(\mathbf{q}) + \varphi' + \Delta). \quad (35)$$

The sum over \mathbf{p} may be calculated in $d = 3$ by approximating (23) as follows

$$\frac{1}{N_s} \sum_{\mathbf{q}} f(\varepsilon(\mathbf{q})) \rightarrow \int_0^1 dq_1 dq_2 dq_3 f(\varepsilon_{\mathbf{q}}), \quad (36)$$

with the lattice dispersion:

$$\varepsilon_{\mathbf{q}} = 2J \sum_{\alpha=1}^3 [1 - \cos \pi q_{\alpha}]. \quad (37)$$

Note that on lattices, the momentum integrals are always finite so that there is no need for renormalizing the coupling constant. This is in contrast to atomic gases. However, if we want to express the coupling constant in terms of the scattering length a_s that is observable at low-energy in atomic gases, where the quadratic coupling constant g must be renormalized to a finite value g_R by the addition of a diverging integral $1/g_R = 1/g + \int d^3p/(2\pi\hbar)^3 \varepsilon(\mathbf{p})$, the relation $a_s = Mg_R/4\pi\hbar^2$ can only be employed only after a corresponding addition of a finite sum [see the remarks after Eq. (92)].

Another remark concerns the frequency sum in (33), which is initially divergent. In fact, to evaluate a frequency sum such as $\sum_{n=-\infty}^{\infty} \ln(a^2 + \omega_n^2)$ with $\omega_n = 2\pi nT$, one must first differentiate it with respect to a , perform the summation over n , and integrate the result over a [31]. This procedure gives an additional divergent constant, which may be removed by an additive renormalization of the energy [32]. The subtraction can actually be justified by calculating the path integral as a product of individual integrals for each slice of a sliced time axis, as introduced in the very beginning by Feynman [31].

In the thermodynamic potential Ω , one subtracts from Ω the one for the “ideal” value

$$\Omega(U = T = 0) = \frac{1}{2} \sum_q (\varepsilon(\mathbf{q}) - \mu - Jz_0) = \frac{1}{2} \sum_q (\varepsilon(\mathbf{q}) + \varphi'), \quad (38)$$

and deals only with the subtrated expression

$$\begin{aligned}\Omega_{\text{ren}} &= \Omega(U, T) - \Omega(U = 0, T = 0) = \frac{1}{2} \sum_{\mathbf{q}} (\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) - \varphi') + N_s \nu n_0 (\varphi' - \Delta) \\ &+ \frac{N_s \Delta^2}{2U \sinh^2 \theta} - \frac{N_s (\varphi' + \mu + Jz_0)^2}{2U \cosh^2 \theta} + T \sum_{\mathbf{q}} \ln(1 - e^{-\beta \mathcal{E}(\mathbf{q})}),\end{aligned}\quad (39)$$

where we have performed summation by Matsubara frequency by using formula

$$\sum_{n=-1}^{\infty} \ln(\omega_n^2 + a^2) = a\beta + 2 \ln(1 - e^{-\beta a}) + \text{divergent constant}.\quad (40)$$

For brevity, we shall suppress writing down the subtraction in Ω_{ren} .

In equilibrium, the thermodynamic potential reaches a minimum with respect to parameters n_0, φ' and Δ . Thus we minimize Ω with respect to n_0

$$\frac{\partial \Omega}{\partial n_0} = N_s \nu (\varphi' - \Delta) = 0,\quad (41)$$

and get

$$\varphi' = \Delta.\quad (42)$$

Inserting this into (35) leads to the well-known Bogoliubov phonon dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})} \sqrt{\varepsilon(\mathbf{q}) + 2\Delta},\quad (43)$$

which is linear in \mathbf{q} for small momentum, thus respecting the Nambu-Goldstone theorem.

Minimizing thermodynamic potential Ω with respect to Δ gives the equation:

$$\Delta = U \sinh^2 \theta \left[\nu n_0 + \frac{\Delta}{N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} \right],\quad (44)$$

where $c_{\mathbf{q}}$ is short for

$$c_{\mathbf{q}} = \frac{1}{2} + f_{\beta}(\mathcal{E}(\mathbf{q})) = \frac{1}{2} \coth(\beta \mathcal{E}(\mathbf{q})/2), \quad f_{\beta}(\omega) = 1/(e^{\beta \omega} - 1).\quad (45)$$

Minimizing Ω with respect to φ' , thereby taking into account the relation $\partial \mathcal{E}(\mathbf{q})/\partial \varphi' = (\varepsilon(\mathbf{q}) + \varphi')/\mathcal{E}(\mathbf{q})$, gives the following equation:

$$N_s \nu n_0 + \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \varphi') c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right] - \frac{N_s (\varphi' + \mu + Jz_0)}{U \cosh^2 \theta} = 0.\quad (46)$$

This will serve to determine of uncondensed fraction $n_{\mathbf{u}}$.

B. Normal and anomalous densities

According to the general rules of statistical mechanics, the total number of particles N is conjugate the chemical potential:

$$N = - \left(\frac{\partial \Omega}{\partial \mu} \right)_{T,V}. \quad (47)$$

Applying this to (39) gives

$$N = \frac{N_s(\varphi' + \mu + Jz_0)}{U \cosh^2 \theta}. \quad (48)$$

Using (48) in (46), we obtain

$$N = N_s \nu n_0 + \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \varphi') c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right] \equiv N_0 + N_{\mathbf{u}}. \quad (49)$$

Here N_0 is a total number of condensed atoms, and $n_0 = N_0/N_s \nu$ is the *condensate fraction*. The uncondensed atoms have a fraction

$$n_{\mathbf{u}} = \frac{N_{\mathbf{u}}}{N} = \frac{1}{\nu N_s} \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \varphi') c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right]. \quad (50)$$

It satisfies the trivial relation $n_0 + n_{\mathbf{u}} = 1$.

Note that, the term $-\frac{1}{2}$ in the square bracket of (50) is due to the renormalization procedure (39), and guarantees that at $T = 0$ all particles of the ideal gas (which has $U = 0$ and $\Delta = 0$) are condensed, so that $n_{\mathbf{u}}(U = 0, T = 0) = 0$.

If the U(1) gauge symmetry is broken, a Bose system is characterized not only by the expectation values of the fluctuating part of the ψ -field with the normal density $n_{\mathbf{u}} = \langle \tilde{\psi}^* \tilde{\psi} \rangle$, but also with anomalous density, defined by

$$\delta(x_{\mathbf{i}}, \tau, x_j, \tau') = \langle \tilde{\psi}(x_{\mathbf{i}}, \tau) \tilde{\psi}(x_j, \tau') \rangle. \quad (51)$$

Clearly, for homogenous system in the equilibrium, in particular, for periodic optical lattices without magnetic trap, δ does not depend on coordinates, i.e. $\delta(x_{\mathbf{i}}, \tau, x_j, \tau') = \text{const}$ as was emphasized in [33]. Omission of the anomalous averages makes all calculations not self-consistent, the dynamics non-conserving, the thermodynamics incorrect. It ruins the order of the phase transition and renders the system unstable. It was also shown in [33] that a $\delta = 0$ type of mean-field approach referred in the literatures as Hartree-Fock-Popov (HFP) approximations [19] leads to a discontinuity in the magnetization curve of antiferromagnetic material with triplon BEC. Thus we must always allow for $\delta \neq 0$.

Let us calculate this expectation value from the formula

$$\begin{aligned}\delta &= \frac{1}{\nu} \langle \tilde{\psi}(x_{\mathbf{i}}, \tau) \tilde{\psi}(x_{\mathbf{i}}, \tau) \rangle = \frac{1}{2\nu} [\langle \tilde{\psi}_1(x_{\mathbf{i}}, \tau) \tilde{\psi}_1(x_{\mathbf{i}}, \tau) \rangle - \langle \tilde{\psi}_2(x_{\mathbf{i}}, \tau) \tilde{\psi}_2(x_{\mathbf{i}}, \tau) \rangle] \\ &= \frac{1}{2\nu} [G_{11}(0) - G_{22}(0)].\end{aligned}\tag{52}$$

In momentum space, the propagator can be rewritten as

$$G_{ab}(\omega_n, \mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} \begin{pmatrix} \varepsilon(\mathbf{q}) + 2\Delta & \omega_n \\ -\omega_n & \varepsilon(\mathbf{q}) \end{pmatrix},\tag{53}$$

where we used equations (21), (25), and (43). Using in (52) the equations (29) and (53), one obtains

$$\delta = \frac{1}{2\nu N_s \beta} \sum_n \sum_{\mathbf{q}} \frac{2\Delta}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} = \frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} = \frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{1}{\mathcal{E}(\mathbf{q})} \left(\frac{1}{2} + \frac{1}{e^{\beta \mathcal{E}(\mathbf{q})} - 1} \right).\tag{54}$$

In terms of δ , the Δ -equation (44) may be rewritten in the following compact form

$$\Delta = U\nu(n_{\mathbf{0}} + \delta) \sinh^2 \theta,\tag{55}$$

with $n_{\mathbf{0}} = 1 - n_{\mathbf{u}}$, and $n_{\mathbf{u}}$ given by (50).

It is well known that the Goldstone theorem for a dilute Bose gas with a spontaneous broken symmetry is equivalent to the celebrated Hugenholtz-Pines theorem [34], according to which self-energy Σ_{cl} and the anomalous self-energy Δ_{cl} satisfy

$$\Sigma_{\text{cl}} - \Delta_{\text{cl}} = \mu.\tag{56}$$

In the Appendix A we shall show that a similar equation holds for optical lattices:

$$\Sigma_{\text{cl}} - \Delta_{\text{cl}} = \mu + Jz_0,\tag{57}$$

with $\Sigma_{\text{cl}} = \varphi_0 \cosh \theta$, $\Delta_{\text{cl}} = \Delta$.

The only parameter, that so far remains free in the initial action (11), is θ . It may be chosen such that the quasiparticle energy $\mathcal{E}(\mathbf{q})$ reduces, in the one-loop approximation [13], to the gapless Bogoliubov dispersion

$$\mathcal{E}(\mathbf{q})_{\text{oneloop}} = \sqrt{\varepsilon(\mathbf{q})} \sqrt{\varepsilon(\mathbf{q}) + 2U\nu}.\tag{58}$$

Indeed, in this approximation we get from (55) $\Delta \approx U\nu \sinh^2 \theta$, and from (43) $\mathcal{E}(\mathbf{q}) \approx \sqrt{\varepsilon(\mathbf{q})} \sqrt{\varepsilon(\mathbf{q}) + 2U\nu \sinh^2 \theta}$. And this is the place where we fix the θ to satisfy

$$\sinh^2 \theta = 1, \quad \cosh^2 \theta = 2,\tag{59}$$

as was announced earlier.

Summarizing this section, we present the full expression for Ω :

$$\Omega = \frac{1}{2} \sum_{\mathbf{q}} [\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) - \Delta] + \frac{N_s \Delta^2}{2U} - \frac{N_s (\Delta + \mu + Jz_0)^2}{4U} + T \sum_{\mathbf{q}} \ln(1 - e^{-\beta \mathcal{E}(\mathbf{q})}), \quad (60)$$

with

$$\mu = 2\nu U - \Delta - Jz_0. \quad (61)$$

The last equation follows from (48). The self energy Δ in (60) and (61) is defined through the following set of nonlinear algebraic equations:

$$\begin{aligned} \Delta &= U\nu(n_0 + \delta), \quad n_0 = 1 - n_{\mathbf{u}}, \\ n_{\mathbf{u}} &= \frac{1}{\nu N_s} \sum_{\mathbf{q}} \left[\frac{c_{\mathbf{q}}(\varepsilon(\mathbf{q}) + \Delta)}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right], \\ \delta &= \frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \end{aligned} \quad (62)$$

where $c_{\mathbf{q}}$ is given in (45) and U, J, ν, T are input parameters.

C. Symmetric phase

When $n_0 = 0$, the Hamiltonian (1) is symmetric under the transformation $\psi \rightarrow e^{i\alpha} \psi$ and equation (41) makes no sense. Then $\varphi' \neq \Delta$, and the energy spectrum has a gap with the dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{(\varepsilon(\mathbf{q}) + \varphi' - \Delta)(\varepsilon(\mathbf{q}) + \varphi' + \Delta)}. \quad (63)$$

The main equations in this regime with $T > T_c$ are

$$\Delta = U\nu\delta, \quad \delta = \frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \quad \nu = \frac{1}{N_s} \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \varphi')c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right]. \quad (64)$$

The set of equations (64) with the energy spectrum (63) may have a solution $\Delta \neq 0, \varphi > \Delta$, leading to an exotic state with no condensate but with a finite anomalous density: $n_0 = 0, \delta \neq 0$. It was shown in Ref. [18] that this phase has a nonzero SF transition. The upper boundary of such a state was denoted by T^* , and was determined by solving the equations (64) with $\Delta = 0, \varphi' > 0$. Thus it was predicted that dilute atomic gases possess a state with $T_c < T^*$ that is a superfluid but has no condensate. However, experimentally, the states with $T > T^*$ are normal with $\delta = 0$ and $n_0 = 0$. In Sect. IV we shall investigate the possible existence of such a state for optical lattices, with a negative outcome.

III. VARIATIONAL PERTURBATION THEORY IN OPTICAL LATTICES

Let us compare our result with those of Variational Perturbation Theory [26]. To lowest order, this is equivalent to the HFB approximation used in the operator formalism [35]. To do this, let us formulate the HFB approximation for optical lattices in the functional integral framework.

Starting point is again (1) in which we perform the Bogoliubov shift (13) and separate it as follows

$$\mathcal{A} = \mathcal{A}_{(0)} + \mathcal{A}_{(1)} + \mathcal{A}_{(2)} + \mathcal{A}_{(3)} + \mathcal{A}_{(4)}, \quad (65)$$

where

$$\begin{aligned} \mathcal{A}_{(0)} &= \beta N_s \nu n_0 \left[\frac{U}{2} \nu n_0 - \mu - J z_0 \right], \\ \mathcal{A}_{(1)} &= \sqrt{\nu n_0} [-\mu - J z_0 + U \nu n_0] \int d\tau \sum_{\mathbf{i}} (\tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau) + \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau)), \\ \mathcal{A}_{(2)} &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{i}} \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) [\partial_\tau - \mu] \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau) + \frac{U}{2} \nu n_0 \right. \\ &\quad \times \sum_{\mathbf{i}} \left[\tilde{\psi}^2(\mathbf{x}_{\mathbf{i}}, \tau) + 4 \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau) + \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \right] - J \sum_{\langle i, j \rangle} \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{j}}, \tau) \left. \right\}, \\ \mathcal{A}_{(3)} &= U \sqrt{\nu n_0} \int_0^\beta d\tau \sum_{\mathbf{i}} [\tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}^2(\mathbf{x}_{\mathbf{i}}, \tau) + \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau)], \\ \mathcal{A}_{(4)} &= \frac{U}{2} \int_0^\beta d\tau \sum_{\mathbf{i}} [\tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau)]^2. \end{aligned} \quad (66)$$

After this we add and subtract following terms

$$\mathcal{A}_{(\Sigma)} = \int_0^\beta d\tau \sum_{\mathbf{i}} \left\{ \Sigma_{\text{cl}} \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau) + \frac{1}{2} \Delta_{\text{cl}} [\tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}^*(\mathbf{x}_{\mathbf{i}}, \tau) + \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau) \tilde{\psi}(\mathbf{x}_{\mathbf{i}}, \tau)] \right\}, \quad (67)$$

with variational parameters Σ_{cl} and Δ_{cl} . The subscripts cl emphasize that these are variational parameters which, in contrast to the earlier fields φ and Δ , are not meant to be functionally integrated.

Using again real and imaginary parts of the complex fields $\tilde{\psi}$, $\tilde{\psi}^*$ as in (16), we rewrite \mathcal{A} as

$$\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_{\text{free}} + \mathcal{A}_{\text{int}}, \quad (68)$$

where

$$\begin{aligned}
\mathcal{A}_{\text{free}} &= \frac{1}{2} \int_0^\beta d\tau \sum_{\mathbf{i}} \sum_{a,b=1,2} \psi_a(\mathbf{x}_{\mathbf{i}}, \tau) [i\varepsilon_{ab} \partial_\tau + Y_a \delta_{ab}] \psi_b(\mathbf{x}_{\mathbf{i}}, \tau), \\
\mathcal{A}_{\text{int}} &= \mathcal{A}_{\text{int}}^{(2)} + \mathcal{A}_{\text{int}}^{(3)} + \mathcal{A}_{\text{int}}^{(4)}, \\
\mathcal{A}_{\text{int}}^{(2)} &= \frac{1}{2} \int_0^\beta d\tau \sum_{\mathbf{i}} \left\{ \psi_1^2(\mathbf{x}_{\mathbf{i}}, \tau) [3U\nu n_{\mathbf{0}} - \Sigma_{\text{cl}} - \Delta_{\text{cl}}] + \psi_2^2(\mathbf{x}_{\mathbf{i}}, \tau) [U\nu n_{\mathbf{0}} - \Sigma_{\text{cl}} + \Delta_{\text{cl}}] \right\}, \\
\mathcal{A}_{\text{int}}^{(3)} &= \frac{1}{2} U \sqrt{2\nu n_{\mathbf{0}}} \int_0^\beta d\tau \sum_{\mathbf{i}} [\psi_1^3(\mathbf{x}_{\mathbf{i}}, \tau) + \psi_1(\mathbf{x}_{\mathbf{i}}, \tau) \psi_2^2(\mathbf{x}_{\mathbf{i}}, \tau)], \\
\mathcal{A}_{\text{int}}^{(4)} &= \frac{1}{8} U \int_0^\beta d\tau \sum_{\mathbf{i}} [\psi_1^2(\mathbf{x}_{\mathbf{i}}, \tau) + \psi_2^2(\mathbf{x}_{\mathbf{i}}, \tau)]^2,
\end{aligned} \tag{69}$$

where

$$\begin{aligned}
Y_1 &= -\mu - Jz_0 + \Sigma_{\text{cl}} + \Delta_{\text{cl}}, \\
Y_2 &= -\mu - Jz_0 + \Sigma_{\text{cl}} - \Delta_{\text{cl}}.
\end{aligned} \tag{70}$$

The free part of the action, $\mathcal{A}_{\text{free}}$ in Eq. (69), gives rise to the propagators to be used in perturbation expansions. In the momentum representation of the fields Eq. (22), the propagator is given by

$$G(\omega_n, \mathbf{q}) = \frac{1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})} \begin{pmatrix} \varepsilon_{\mathbf{q}} + Y_2 & \omega_n \\ -\omega_n & \varepsilon_{\mathbf{q}} + Y_1 \end{pmatrix}, \tag{71}$$

with $\mathcal{E}^2(\mathbf{q}) = (\varepsilon_{\mathbf{q}} + Y_1)(\varepsilon_{\mathbf{q}} + Y_2)$. To lowest order, one obtains

$$\Omega = -T \ln Z = -T \ln Z_0 - T \ln Z_{\text{free}} + T \langle \mathcal{A}_{\text{int}} \rangle, \tag{72}$$

where $Z_0 = e^{-\mathcal{A}_0}$, $Z_{\text{free}} = \int \mathcal{D}\psi_1 \mathcal{D}\psi_2 e^{-\mathcal{A}_{\text{free}}} = 1/\sqrt{\text{Det } G^{-1}}$, $\langle \mathcal{A}_{\text{int}} \rangle = \int \mathcal{D}\psi_1 \mathcal{D}\psi_2 \mathcal{A}_{\text{int}} e^{-\mathcal{A}_{\text{free}}}$.

Now we evaluate

$$\langle \psi_a^2(\mathbf{x}_{\mathbf{i}}, \tau) \rangle = G_{aa}(0) = \frac{B_a}{N_s}, \quad \langle \psi_a^4(\mathbf{x}_{\mathbf{i}}, \tau) \rangle = \frac{3\sigma_a^2}{N_s^2}, \quad \langle \psi_1^2(\mathbf{x}_{\mathbf{i}}, \tau) \psi_2^2(\mathbf{x}_{\mathbf{i}}, \tau) \rangle = \frac{\sigma_1 \sigma_2}{N_s^2}, \tag{73}$$

with

$$\sigma_1 = T \sum_{\mathbf{q}, n} \frac{\varepsilon_{\mathbf{q}} + Y_2}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})}, \quad \sigma_2 = T \sum_{\mathbf{q}, n} \frac{\varepsilon_{\mathbf{q}} + Y_1}{\omega_n^2 + \mathcal{E}^2(\mathbf{q})}, \tag{74}$$

and we find the following thermodynamic potential:

$$\begin{aligned}
\Omega &= N_s \nu n_{\mathbf{0}} \left(-\mu - Jz_0 + \frac{U}{2} \nu n_{\mathbf{0}} \right) + \frac{1}{2} \sum_{\mathbf{q}} [\mathcal{E}(\mathbf{q}) - \varepsilon(\mathbf{q}) + \mu + Jz_0] \\
&\quad + T \sum_{\mathbf{q}} \ln(1 - e^{-\beta \mathcal{E}(\mathbf{q})}) + \frac{U\nu}{8N} [3\sigma_1^2 + 3\sigma_2^2 + 2\sigma_1 \sigma_2] \\
&\quad + \frac{1}{2} \sigma_1 (3U\nu n_{\mathbf{0}} - Y_1 - Jz_0 - \mu) + \frac{1}{2} \sigma_2 (U\nu n_{\mathbf{0}} - Y_2 - Jz_0 - \mu),
\end{aligned} \tag{75}$$

where we have again subtracted $\Omega(T=0, U=0)$.

The parameters Σ_{cl} and Δ_{cl} are now determined variationally by requiring that they minimize the thermodynamic potential, i.e., we require $\partial\Omega/\partial\Sigma_{\text{cl}} = 0$ and $\partial\Omega/\partial\Delta_{\text{cl}} = 0$ [36], or equivalently

$$\frac{\partial\Omega}{\partial Y_1} = 0, \quad \frac{\partial\Omega}{\partial Y_2} = 0. \quad (76)$$

These equations yield

$$\begin{aligned} Y_1 &= 3U\nu n_{\mathbf{0}} - \mu - Jz_0 + \frac{U}{2N_s}(3\sigma_1 + \sigma_2), \\ Y_2 &= U\nu n_{\mathbf{0}} - \mu - Jz_0 + \frac{U}{2N_s}(\sigma_1 + 3\sigma_2). \end{aligned} \quad (77)$$

The gaplessness of the energy spectrum is now imposed by hand. In fact, by requiring the relation (57), we get from (70) $Y_2 = 0$ which leads to the dispersion

$$\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})} \sqrt{\varepsilon(\mathbf{q}) + 2\Delta}, \quad (78)$$

where $\Delta = Y_1/2$. This leads to the equations

$$\begin{aligned} \Delta &= U\nu n_{\mathbf{0}} + \frac{U}{2N_s}(\sigma_1 - \sigma_2), \\ \mu + Jz_0 &= U\nu n_{\mathbf{0}} + \frac{U}{2N_s}(\sigma_1 + 3\sigma_2). \end{aligned} \quad (79)$$

Here, we draw the reader's attention to the inself-consistency of the HFB approximation as far as the chemical potential is concerned. In fact, the stationary condition $\partial\Omega/\partial n_{\mathbf{0}} = 0$ with Ω given by (75) leads to the following equation for μ :

$$\mu + Jz_0 = U\nu n_{\mathbf{0}} + \frac{U}{2N_s}(3\sigma_1 + \sigma_2), \quad (80)$$

which contradicts μ of Eq. (79).

To make the theory self-consistent, Yukalov and one of the authors [37] proposed to introduce two chemical potentials: namely, μ_0 , which corresponds to the Eq. (80), and μ_1 corresponding to Eq. (79). Being responsible for subsystem of condensed and uncondensed particles they, naturally, coincide in the normal phase, when $Y_1 = Y_2 = 0$. In the present work, however, we follow the standard procedure of identifying μ in (79) as a chemical potential from which we determine the particle densities by differentiation of Ω .

A. The fractions $n_{\mathbf{u}}$ and δ in VPT

Applying the well-known relation $N = -\partial\Omega/\partial\mu$ to Ω in (75) gives

$$N = N_s\nu n_{\mathbf{0}} + \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \Delta)c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right] \equiv n_{\mathbf{0}} + n_{\mathbf{u}}, \quad (81)$$

and hence

$$n_{\mathbf{u}} = \frac{n_{\mathbf{u}}}{N_s} = \frac{1}{\nu N_s} \sum_{\mathbf{q}} \left[\frac{(\varepsilon(\mathbf{q}) + \Delta)c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})} - \frac{1}{2} \right], \quad (82)$$

with the $\mathcal{E}(\mathbf{q})$ is the Bogoliubovs dispersion given in (78).

For the anomalous density δ we obtain

$$\begin{aligned} \delta &= \frac{1}{\nu} \langle \tilde{\psi}(\mathbf{x}_i, \tau) \tilde{\psi}(\mathbf{x}_i, \tau) \rangle = \frac{1}{2N_s \beta \nu} [G_{11}(0) - G_{22}(0)] = \frac{(\sigma_1 - \sigma_2)}{2N_s \nu} \\ &= -\frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \end{aligned} \quad (83)$$

where we used Eqs. (71) and (74).

Using now (83) in (79) gives the equation:

$$\Delta = U\nu(n_0 + \delta), \quad (84)$$

which is the same as the one in before (55) with (59). The only difference between these two approximations is in the sign of anomalous density, which is $\delta > 0$ in the collective quantum field theory and $\delta < 0$ in HFB.

Summarizing we collect here the main equations in both approximations:

$$\Delta = U\nu(n_0 + \delta), \quad n_0 = 1 - n_{\mathbf{u}}, \quad (85)$$

$$\delta = \xi \frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}, \quad \mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})} \sqrt{\varepsilon(\mathbf{q}) + 2\Delta}, \quad c_{\mathbf{q}} = \frac{1}{2} + \frac{1}{e^{\beta \mathcal{E}(\mathbf{q})} - 1}, \quad (86)$$

$$\mu = 2U\nu - \Delta - Jz_0, \quad (87)$$

$$\xi = \begin{cases} -1, & \text{HFB} \\ +1, & \text{Two Collective Quantum Fields.} \end{cases} \quad (88)$$

Note that similar relations hold for atomic gases. A difference occurs for the $T > T_c$ phase. There one must use replacements listed in Appendix B. In fact, in the normal phase, $n_0 = 0$, HFB theory gives

$$\Delta = U\nu\delta = -\frac{\Delta}{\nu N_s} \sum_{\mathbf{q}} \frac{c_{\mathbf{q}}}{\mathcal{E}(\mathbf{q})}. \quad (89)$$

Since the right-hand-side of this equation is positive, while the left-hand-side is negative, at least for optical lattices, Eq. (89) has as only solution $\Delta = 0$ [see Eq. (86)]. This means that in the normal phase $n_0 = 0$ and $\delta = 0$ simultaneously. Therefore HFB theory does not predict a superfluid phase without a condensate, this being in contrast to the two-collective quantum field result of Cooper et.al. in Ref. [18] at the mean-field level.

From above discussions it is easy to understand that VPT gives no shift in T_c due to interaction. In fact, when $T \rightarrow T_c$, the condensed fraction $n_0 \rightarrow 0$, and hence $\Delta \rightarrow 0$. The expression for n_u , will coincide with that for the ideal gas, i.e., Eq. (82) becomes

$$\nu = \frac{1}{N_s} \sum_{\mathbf{q}} \frac{1}{e^{\beta \varepsilon(\mathbf{q})} - 1} \equiv \frac{1}{N_s} \sum_{\mathbf{q}} \frac{1}{e^{\varepsilon(\mathbf{q})/T_c^0} - 1}, \quad (90)$$

which means that $T_c = T_c^0$ for HFB and, hence, $\Delta T_c = T_c - T_c^0 = 0$.

IV. RESULTS AND DISCUSSION

A. Quantum phase transition in two-Collective Quantum Field Theory and VPT

First we discuss the existence of QPT in optical lattices for two collective quantum fields at the mean field level and for the HFB approximation. It has been shown that for dilute atomic Bose gases Collective Quantum Field approximation does not predict QPT [15] while HFB does [33]. Below we show that in the case of $3d$ optical lattices the situation is vice-versa. This can be understood in the following way. Lets rewrite main equation at $T = 0$ as:

$$n_0(\Delta) = \frac{\Delta}{U\nu} - \delta(\Delta). \quad (91)$$

It is clear that for interacting system, $U \neq 0$ and $\Delta \neq 0$. Since in the collective quantum field theory $\delta(\Delta) > 0$, the Eq. (91) may have solution $n_0(\Delta) = 0$ with $\Delta \neq 0$ (see Table I). However, in HFB approximation $\delta(\Delta) < 0$ and $n_0(\Delta)$ in (91) may have only solution as $n_0 > 0$ for $\Delta \neq 0$. Note that in the case of dilute atomic gases

$$\begin{aligned} \delta(\Delta) &= -8\rho\sqrt{\gamma/\pi} < 0 \quad \text{two-Collective Quantum Field Theory} \\ \delta(\Delta) &= +8\rho\sqrt{\gamma/\pi} > 0 \quad \text{HFB,} \end{aligned} \quad (92)$$

with the dimensionless *gas parameter* $\gamma = a_s^3\rho$ that characterized the interaction strength of the gas after renormalization. It is formed from the s -wave scattering length a_s and the particle density ρ . This sign change is responsible for the dilute atomic gases has a QPT in the HFB approximation, but not in the two-collective quantum field theory at the mean-field level.

TABLE I: Critical parameter $u_c = (U/J)_c$ of QPT in the two collective quantum field approach. The critical temperatures of ideal optical lattices in $d = 3$ are listed (in units J). The third row presents approximated values of t_c^0 [see Eq. (95)]

ν	1	2	3	4	5
$u_c = (U/J)_c$	28.04	47.70	67.15	82.52	105.91
$t_c^0 = T_c^0/J$	5.6	9.69	13.70	17.70	21.67
t_c^0 in small q approximation	5.06	10.07	15.2	20.25	25.32

B. Critical temperature T_c^0 for ideal cases

Before we study the shift of T_c , let us estimate the critical temperature T_c^0 for the free optical lattice with $U = 0$. Assuming $\Delta = 0$ in Eq. (64), we obtain the well-known formula

$$\nu = \int_0^1 dq_1 dq_2 dq_3 \frac{1}{e^{\varepsilon_{\mathbf{q}}/T_c^0} - 1}. \quad (93)$$

Introducing dimensionless parameters $t_c^0 = T_c^0/J$, $\hat{\varepsilon}_{\mathbf{q}} = \varepsilon_{\mathbf{q}}/2J = \sum_{\alpha=1}^3 (1 - \cos \pi q_{\alpha})$, we may rewrite (93) as

$$\nu = \int_0^1 dq_1 dq_2 dq_3 \frac{1}{e^{2\hat{\varepsilon}_{\mathbf{q}}/t_c^0} - 1} \quad (94)$$

which can be considered as a nonlinear equation for t_c^0 at a given filling factor ν . Our numerical estimations for t_c^0 are given in Table I. It is seen that for $\nu = 1$, $T_c^0 = 5.6J$, which is consistent with other estimates given in the references [3, 10].

Note that T_c^0 can be approximated as $T_c^0 = 5.6J\nu^{0.825}$ in the range $\nu \in (1, 5)$ including also non integer values. In the third row of Table 1 an approximated values of t_c^0 are presented. This approximation, say, spherical approximation at for small momentum is obtained by following replacements in (94):

$$\begin{aligned} \int_0^1 dq_1 dq_2 dq_3 f(\mathbf{q}) &\rightarrow \frac{\pi}{2} \int_0^{q_d} q^2 dq f(q), \\ \hat{\varepsilon}_{\mathbf{q}} &\rightarrow \frac{\pi^2}{2} \mathbf{q}^2, \quad (e^{\varepsilon_{\mathbf{q}}/T_c^0} - 1)^{-1} \rightarrow \frac{T_c^0}{\varepsilon(\mathbf{q})}, \end{aligned} \quad (95)$$

where the Debye momentum q_D defined by the equation:

$$1 = \int_0^1 dq_1 dq_2 dq_3 = \frac{\pi}{2} \int_0^{q_d} q^2 dq, \quad (96)$$

equals to $q_d = (6/\pi)^{1/3} \approx 1.24$ for $d = 3$ which gives $T_c^0/J = 2\nu\pi(\pi/6)^{1/3}$. It is seen that this approximation works with roughly 10% accuracy for $\nu \leq 3$.

C. The shift in T_c caused by the interaction

We are now prepared to estimate the shift $\Delta T_c/T_c^0 = (T_c - T_c^0)/T_c^0$ analytically. The integral is dominated by small momenta. The main equations at $T \rightarrow T_c$ for $n_0 = 0$, $n_u = 1$ are

$$\Delta = U\Delta \int_0^1 dq_1 dq_2 dq_3 \frac{f_B(\mathcal{E}(\mathbf{q}))}{\mathcal{E}(\mathbf{q})}, \quad (97)$$

$$1 = \frac{1}{\nu} \int_0^1 dq_1 dq_2 dq_3 \frac{(\varepsilon_{\mathbf{q}} + \Delta)}{\mathcal{E}(\mathbf{q})} f_B(\mathcal{E}(\mathbf{q})), \quad (98)$$

with $\mathcal{E}(\mathbf{q}) = \sqrt{\varepsilon_{\mathbf{q}}} \sqrt{\varepsilon_{\mathbf{q}} + 2\Delta}$, $f_B(\mathcal{E}(\mathbf{q})) = 1/(e^{\beta_c \mathcal{E}(\mathbf{q})} - 1)$, $\beta_c = 1/T_c$.

Note that in (97) we may assume $\Delta \neq 0$ and divide both sides of (97) by Δ . The critical temperature of ideal gas T_c is the solution of Eq. (98) with $\Delta = 0$, i.e.,

$$1 = \frac{1}{\nu} \int_0^1 \frac{dq_1 dq_2 dq_3}{e^{\varepsilon_{\mathbf{q}}/T_c^0} - 1}. \quad (99)$$

Now we introduce dimensionless variables:

$$\Delta = u^2 \kappa^2 T_c^0, \quad T_c = T_c^0 \alpha, \quad T_c^0 = J t_c^0, \quad \varepsilon_{\mathbf{q}} = 2J \hat{\varepsilon}_{\mathbf{q}}, \quad \mathcal{E}(\mathbf{q}) = 2J \hat{\mathcal{E}}(\mathbf{q}), \quad (100)$$

with $\hat{\varepsilon}_{\mathbf{q}} = \sum_{\alpha} (1 - \cos \pi \mathbf{q}_{\alpha})$, $\hat{\mathcal{E}}(\mathbf{q}) = \sqrt{\hat{\varepsilon}_{\mathbf{q}}} \sqrt{\hat{\varepsilon}_{\mathbf{q}} + u^2 \kappa^2 t_c^0}$, $\Delta T_c/T_c^0 = \alpha - 1$ and t_c^0 are given in the third row of Table 1.

The scaled equations can be rewritten as follows:

$$0 = 1 - \frac{u}{2} \int_0^1 \frac{f_B(\hat{\mathcal{E}}(\mathbf{q})) dq_1 dq_2 dq_3}{\hat{\mathcal{E}}(\mathbf{q})}, \quad (101)$$

$$0 = 1 - \frac{\nu}{2} \int_0^1 dq_1 dq_2 dq_3 \frac{\hat{\varepsilon}_{\mathbf{q}} + u^2 \kappa^2 t_c^0/2}{\hat{\mathcal{E}}(\mathbf{q})} f_B(\hat{\mathcal{E}}(\mathbf{q})), \quad (102)$$

with $f_B(\hat{\mathcal{E}}(\mathbf{q})) = 1/(e^{2\hat{\mathcal{E}}(\mathbf{q})/\alpha t_c^0} - 1)$.

Bearing in mind (99), we may rewrite (102) as

$$\int_0^1 dq_1 dq_2 dq_3 \left\{ \frac{1}{e^{2\hat{\mathcal{E}}(\mathbf{q})/t_c^0} - 1} - \frac{\hat{\varepsilon}_{\mathbf{q}} + u^2 \kappa^2 t_c^0/2}{\hat{\mathcal{E}}(\mathbf{q}) (e^{2\hat{\mathcal{E}}(\mathbf{q})/\alpha t_c^0} - 1)} \right\} = 0. \quad (103)$$

The nonlinear equations (101) and (103) should be solved with respect to κ and α with given numbers $u = U/J$ and t_c^0 . To do this we make replacements (95). Then Eqs. (101) and (103) can be rewritten as

$$1 - \frac{u \alpha t_c^0}{4\sqrt{2}\pi^2} \int_0^{\varepsilon_D} \frac{d\varepsilon}{\sqrt{\varepsilon}(\varepsilon + u^2 \kappa^2 t_c^0)} = 0, \quad (104)$$

$$\int_0^{\varepsilon_D} \frac{d\varepsilon}{\sqrt{\varepsilon}} \left\{ 1 - \frac{\alpha(\varepsilon + u^2 \kappa^2 t_c^0/2)}{\varepsilon + u^2 \kappa^2 t_c^0} \right\} = 0, \quad (105)$$

where $\varepsilon_D = \pi^2 q_D^2 / 2 = (\pi^2 / 2)(6/\pi)^{2/3}$

The integrals in (104) and (105) are easily done and yield

$$0 = \sqrt{2}(6\pi^2)^{1/3}(1 - \alpha) + u\alpha\kappa\sqrt{t_c^0} \arctan \tilde{\theta} \quad (106)$$

$$0 = 4\pi^2\kappa - \sqrt{2}\alpha\sqrt{t_c^0} \arctan \tilde{\theta}, \quad (107)$$

where $\tilde{\theta} = \sqrt{2}(6\pi^2)^{1/3}/(2\kappa u\sqrt{t_c^0})$. Excluding α from (107) and inserting it to (106) gives

$$\alpha = \frac{2\sqrt{2}\pi^2\kappa}{\sqrt{t_c^0} \arctan \tilde{\theta}}, \quad (108)$$

$$0 = 4\kappa\pi^{8/3}6^{1/3} - \sqrt{2t_c^0}[(6\pi^2)^{1/3} + 2u\kappa^2\pi^2] \arctan \tilde{\theta}. \quad (109)$$

Now we consider separately two regimes:

a) Weak interacting regime. Expanding (108) and (109) in linear order by u we get

$$\alpha = \frac{4\pi^2\kappa\sqrt{2}}{\sqrt{t_c^0}} + \frac{8\kappa^2u}{3} \left(\frac{6}{\pi}\right)^{2/3}, \quad (110)$$

$$\kappa = \frac{\sqrt{2t_c^0}}{8\pi}. \quad (111)$$

Now inserting κ into (110) we finally obtain

$$\alpha = 1 + \frac{ut_c^0}{12} \left(\frac{6}{\pi^4}\right)^{2/3} + O(u^2), \quad (112)$$

and hence

$$\frac{\Delta T}{T_c^0} = \alpha - 1 = \frac{ut_c^0}{12} \left(\frac{6}{\pi^4}\right)^{2/3} + O(u^2), \quad (113)$$

which means that for small coupling constant, i.e. $(U/J) < 1$, the shift is positive.

b) Strong interacting regime. In this region, Δ/u^2 i.e. κ is small, so we may use a linear approximation in κ in Eqs. (108), (109)

$$\alpha = \frac{4\pi^2\kappa\sqrt{2}}{\sqrt{t_c^0}}, \quad (114)$$

$$0 = \frac{\sqrt{2t_c^0}(6\pi^5)^{1/3}}{2} - \kappa[2ut_c^0 + 4(6\pi^8)^{1/3}]. \quad (115)$$

This leads to following equation

$$\alpha = \frac{2\pi^{8/3}6^{1/3}}{ut_c^0 + 2\pi^{8/3}6^{1/3}} = \frac{T_c}{T_c^0}, \quad (116)$$

from which one may conclude that T_c decreases with increasing u , i.e.

$$\frac{\Delta T_c}{T_c^0} = \alpha - 1 = -\frac{ut_c^0}{ut_c^0 + 2\pi^{8/3}6^{1/3}} < 0. \quad (117)$$

Thus, our analytical estimate shows that the critical temperature T_c as a function of the coupling constant U , i.e. the function $T(u)$ first increases and then decreases with increasing u for optical lattices. This is in good agreement with experimental measurements [4]. Note that, this behavior is in contrast to the case of dilute atomic gases, where the shift is always positive in the whole range of repulsive coupling constant.

In Figure 1 we present T_c (in unit of J) vs. u for $\nu = 1$. The solid line correspond to the exact numerical calculation, i.e., the numerical solutions of Eqs. (97), (98). The experimental points (circles) are taken from [4], solid triangles are from Monte-Carlo calculations taken from ref.[3]

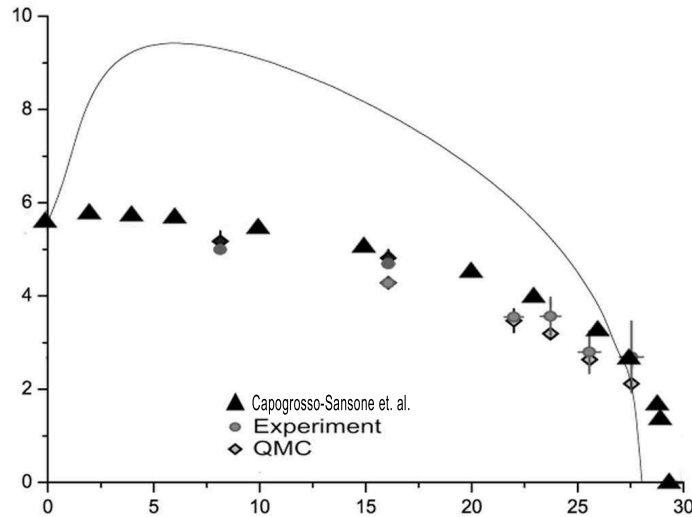


FIG. 1: Behavior of T_c as a function of U/J in the saddle-point approximation to the two-collective field theory for $\nu = 1$. The circles show experimental values given in [4], solid triangles are from Monte-Carlo calculations of Ref. [3]. Note the initial rise that was found also in atomic gases in Ref. [17].

The suppression of T_c at large coupling constant is found for $\nu \geq 1$ as it is also seen in Fig. 2.

In Fig. 3 we present the critical values of the self energy $\Delta_c = \Delta(T = T_c)$ in units J vs. (U/J) . Observe that when J is fixed, Δ_c increases with increasing u and ν . On the other

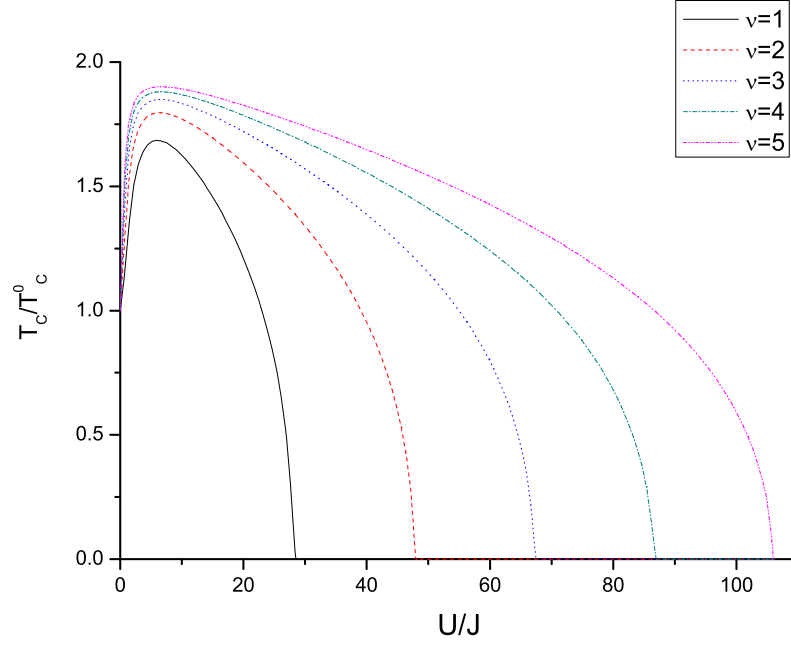


FIG. 2: (Color online) The same curves as in Fig. 1 but for $\nu = 1, 2, 3, 4, 5$.

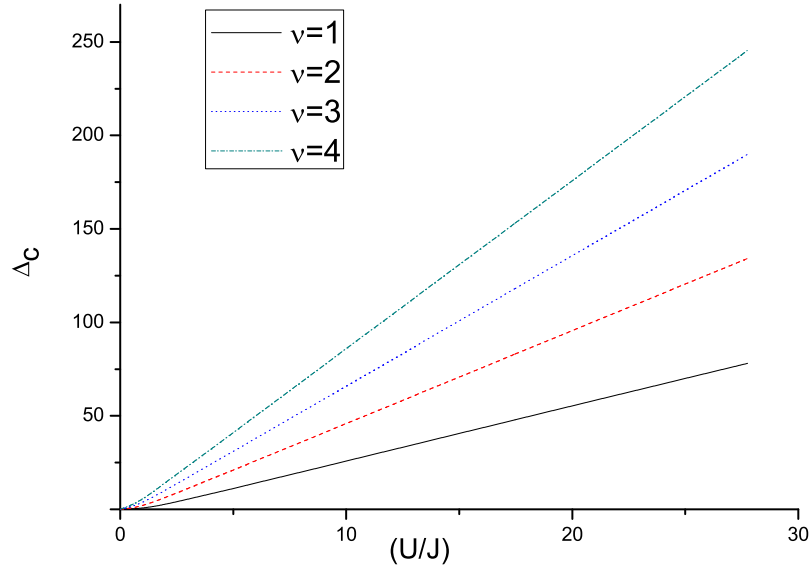


FIG. 3: (Color online) The critical Δ_c vs. u for various filling factors ν .

hand we observed that Δ_c in units $T_c^0(\nu)$, i.e. $\Delta_c(T = T_c)/T_c^0(\nu)$ vs. u is almost independent on ν , e.g., $(\Delta_c/T_c^0)|_{\nu=1} = 10.425$ and $(\Delta_c/T_c^0)|_{\nu=4} = 10.447$ at $u = 21.0$.

Now we consider the behavior of Δ for $T > T_c$. It was suggested by Cooper et.al. [18] that in the temperature range $T \in (T_c, T^*)$ there exists a $U(1)$ -symmetric phase with $n_0 = 0$ but $\delta \neq 0$. This would imply the existence of a superfluid state without a condensate. However, by solving (64) for Δ and φ' , we could not find, for optical lattices, any solution with $\Delta \neq 0, \varphi' \neq 0$. Instead, the equations for $T > T_c$, have a solution with $\Delta = 0, \varphi' = 2U\nu - Jz_0 - \mu$. In this normal state with $\delta = 0$, the filling factor that characterizes the particle density, is determined by the well-known equation

$$\nu = \frac{1}{N_s} \sum_{\mathbf{q}} \frac{1}{e^{\beta(\varepsilon_{\mathbf{q}} - 2U\nu - Jz_0 - \mu)} - 1} = \int_0^1 dq_1 dq_2 dq_3 \frac{1}{e^{\beta(\varepsilon_{\mathbf{q}} - 2U\nu - Jz_0 - \mu)} - 1}, \quad (118)$$

with the bare dispersion $\varepsilon_{\mathbf{q}} = 2J \sum_{\alpha=1}^3 (1 - \cos \pi q_{\alpha})$.

The chemical potential of interacting bosons in $T > T_c$ may be evaluated self consistently from Eq. (118) with input parameters ν , J , U , and T , or given by an external field (pumping) as in the case of triplons [19, 20].

V. CONCLUSION

In this paper we have developed a Collective Quantum Field Theory and a HFB approximations for $d = 3$ optical lattices at very low temperatures. We have shown that, in contrast to the situation in dilute atomic gases, a two-Collective Quantum Field treatment in the saddle point approximation predicts a Quantum Phase transition, that is missed in a HFB approximation. The shift of T_c due to the point interaction is zero for HFB, while it has a nontrivial dependence on the coupling strength (U/J) in the Collective Quantum Field treatment. The latter agrees with experimental observations as well as with Mont-Carlo calculations.

We have found no exotic superfluid state with finite anomalous density but zero condensate. Therefore, the temperatures T^* and T_c introduced by Cooper et.al. [18] coincide. The system is in superfluid state for $0 \leq T \leq T_c$, and in normal state for $T > T_c$. Application of present theory to $d = 1$ and $d = 2$ lattices is in progress.

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Appendix A

Below we derive Hugenholtz-Pines theorem

$$\Sigma_{\text{cl}} - \Delta_{\text{cl}} = \mu + Jz_0, \quad (119)$$

of Sect. II for optical lattices. The normal Σ_{cl} , and anomalous Δ_{cl} self-energies in (119) correspond to the normal $G_{\text{n}}(r, r') = \langle T_{\tau} \tilde{\Psi}(r) \tilde{\Psi}^+(r') \rangle$ and anomalous $G_{\text{an}}(r, r') = -\langle T_{\tau} \tilde{\Psi}(r) \tilde{\Psi}(r') \rangle$ Green functions respectively. In the field representation (16) we have:

$$\Sigma_{\text{cl}} = \frac{1}{2}[\Pi_{11} + \Pi_{22}], \quad (120)$$

$$\Delta_{\text{cl}} = \frac{1}{2}[\Pi_{22} - \Pi_{11}], \quad (121)$$

where Π_{ab} are defined by Dyson-Beliaev equations [38]:

$$(\hat{G}^{-1})_{ab} - (\hat{G}_0^{-1})_{ab} = \Pi_{ab}, \quad (122)$$

and the Green function \hat{G}_0 corresponds to the noninteracting situation

$$G_0^{-1}(\omega_n, \mathbf{q}) = \begin{pmatrix} \varepsilon(\mathbf{q}) - \mu - Jz_0 & -\omega_n \\ \omega_n & \varepsilon(\mathbf{q}) - \mu - Jz_0 \end{pmatrix}. \quad (123)$$

The interacting Green function \hat{G}^{-1} is defined in Eq.(25). Using (21), (34), (25), (123) in (122) gives:

$$\begin{aligned} \Pi_{11} &= X_1 + \mu = \cosh \theta \varphi_0 - \Delta, \\ \Pi_{22} &= X_2 + \mu = \cosh \theta \varphi_0 + \Delta, \\ \Pi_{12} &= \Pi_{21} = 0. \end{aligned} \quad (124)$$

Inserting (124) into (120) and (121) one derives

$$\begin{aligned} \Sigma_{\text{cl}} &= \varphi_0 \cosh \theta, \\ \Delta_{\text{cl}} &= \Delta. \end{aligned} \quad (125)$$

and hence

$$\Sigma_{\text{cl}} - \Delta_{\text{cl}} = \varphi_0 \cosh \theta - \Delta = \varphi' + \mu + Jz_0 - \Delta, \quad (126)$$

where we have used Eq.(34). As it has been shown in Sect. II, in the condensed phase $\varphi' = \Delta$ and Eq.(126) becomes equivalent to the Hugenholtz-Pines theorem, i.e. to Eq.(119).

The relation (119) in HFB approximation can be proved in a similar way.

Appendix B

Here we present formal equivalence between Bose-Hubbard Hamiltonian (1) in Wannier representation and standard Hamiltonian for homogeneous dilute atomic gases

$$H = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[-\frac{\vec{\nabla}^2}{2m} - \mu \right] \Psi(\mathbf{r}) + \frac{g}{2} \int d\mathbf{r} [\Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r})]^2, \quad (127)$$

where g is the constant of contact interatomic interaction. Using the replacements listed in Table II we obtain for Ω and the extremality equations in dilute atomic gases versus optical lattices the relevant quantities as derived in Sections II and III. Of course, an appropriate renormalization procedure is implied in dilute atomic gases.

TABLE II: Formal similarity between Hamiltonian (1) and (127)

Quantity	Atomic gases	3D optical lattices	Comment
Volume	V	N_s	N_s – number of states
Density	$\rho = N/V$	$\nu = N/N_s$	ν – filling factor
Bare dispersion	$\varepsilon(\mathbf{q}) = \mathbf{q}^2/2m$	$\varepsilon(\mathbf{q}) = 2J \sum_{\alpha=1}^3 (1 - \cos \pi q_\alpha)$	no additional magnetic trap
Chemical potential	μ	$\mu + Jz_0$	$N = - \left(\frac{\partial \Omega}{\partial \mu} \right)$
Momentum summation	$\sum_q f(\varepsilon(\mathbf{q})) = 4\pi \int_0^\infty q^2 dq f(\varepsilon(q))$	$\sum_q f(\varepsilon(\mathbf{q})) = \int_0^1 dq_1 dq_2 dq_3 f(\varepsilon(q))$	
Normalization of densities	$\rho_0 + \rho_1 = \rho$	$n_0 + n_1 = 1$	

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- [1] O. Morsch and M. Oberthaler Rev. Mod. Phys. **78**, 179 (2006).
 - [2] R. Raussendorf, D.E. Browne and H. J. Briegel, Phys. Rev. A **68**, 022312 (2003).
 - [3] B. Capogrosso-Sansone, N. V. Prokofiev, and B. V. Svistunov, Phys. Rev. **B** 75, 134302 (2007).
 - [4] Trotzky, L. Pollet, F. Gerbier, U. Schnorrberger, I. Bloch, N. V. Prokofiev, B. Svistunov and M. Troyer, Nature Phys. **6**, 998 (2010).
 - [5] F. E. A. dos Santos and A. Pelster, Phys. Rev. A **79**, 013614 (2009).
 - [6] H. T. C. Stoof, K. B. Gubbels and D.B.M. Dickerscheid *Ultracold Quantum Fields* (Springer, 2009).
 - [7] M. G. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963)
 - [8] D. S. Rokhsar and B. G. Kotliar Phys. Rev. B **44**, 10328 (1991) ;
D. Jaksch, C. Bruder, et al. Phys. Rev. Lett. **81**, 3108 (1998).
 - [9] W. Krauth , M. Caffarel, and J. Bouchaud Phys. Rev. B **45**, 3137 (1992)

- [10] V. I. Yukalov, Laser Physics **19**, 1 (2009).
- [11] P. Buonsante and A. Vezzani, Phys. Rev. A **70**, 033608 (2004).
- [12] D. van Osten, O. van der Straten and H.T.C. Stoof Phys. Rev. A **63**, 053601 (2001).
- [13] H. Kleinert, Z. Narzikulov, Abdulla Rakhimov Phys. Rev. A **85**, 063602 (2012).
- [14] F. Cooper, B. Mihaila, et al. Phys. Rev. A **83**, 053622 (2011).
- [15] B. Mihaila, F. Cooper, et al. Phys. Rev. A **84**, 023603 (2011).
- [16] G. Baym and G. Grinstein, Phys. Rev. D **15**, 2897 (1997).
- [17] H. Kleinert, Mod. Phys. Lett. B **17**, 1011 (2003) (klrt.de/320).
- [18] J.F. Dawson, B. Mihaila, and F. Cooper, Phys. Rev. A **86**, 013603 (2012).
- [19] Abdulla Rakhimov, S. Mardonov, and E. Ya. Sherman, Annals of Phys. **326**, 2499 (2011).
- [20] Abdulla Rakhimov, et al. New J. Phys. **14**, 113010 (2012).
- [21] For field theories on a lattice see H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I Superflow and Vortex Lines, World Scientific, Singapore 1989 (klrnt.de/b1).
- [22] H. Kleinert, Fortschr. Phys. **26**, 565 (1978) (klrnt.de/55).
- [23] H. Kleinert, *Collective Classical and Quantum Fields*, World Scientific, Singapore, 2013 (klrnt.de/b7).
- [24] H. Kleinert, Fortschr. Phys. **30**, 187 (1982).
- [25] R.P Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).
- [26] H. Kleinert and Schulte-Frohlinde, *Critical Properties of Φ^4 -Theories*, World Scientific, Singapore 2001 (klrnt.de/b8).
- [27] H. Kleinert, EJTP **8**, 15 (2011) (klrnt.de/387).
- [28] H. Kleinert, EJTP **8**, 25 (2011) (klrnt.de/391).
- [29] I. Danshita and P. Naidon, Phys. Rev. A **79**, 043601 (2009).
- [30] See Section 4.3 in Ref. [31].
- [31] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, World Scientific Publishing Co., Singapore 1995 (klrnt.de/b5). See the discussion in Subect. 2.15.2.
- [32] T. Haugset, H. Haugerud and F. Ravndal, Ann. Phys. **27**, 266 (1998).
- [33] V. I. Yukalov Ann. Phys. **323**, 461 (2008).
- [34] W. H. Dickhoff and D. Van Neck, *Many-Body Theory Exposed* World Scientific (2005).
- [35] J. O. Andersen, Rev. Mod. Phys. **76**, 599 (2004).
- [36] H. Kleinert, EJTP **8**, 57 (2011) (klrnt.de/391).

- [37] V. I. Yukalov, H. Kleinert, Phys. Rev. A **73**, 063612 (2006).
- [38] H. Shi and A. Griffin, Phys.Rep. 304, 1 (1998).